PARAMETER ESTIMATION AND MULTI-SCALE SIMULATIONS OF SURFACE ROUGHNESS EVOLUTION DURING COPPER ELECTRODEPOSITION

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Copper electrodeposition is currently used for on-chip interconnections due to low cost, good electromigration performance, and ability to fill damascene structures void-free[1]. A fundamental understanding of the molecular-scale influence of additives on the deposition process at the cathode surface is key to achieving improved system performance.

The goal of this presentation is to report on computational tools that accurately simulate the deposition process, particularly the influence of additives on surface roughness evolution and trench in-fill.

In this work, we present two computational tools developed to compliment experimental studies traditionally used to analyze complex additive systems. The first computational tool is an externally linked continuum/non-continuum model that simulates surface roughness evolution. The continuum finite difference code considers transport phenomena in the diffusion boundary layer near the surface. The non-continuum Monte Carlo code uses copper and additive pseudo-particles to simulate the growth of deposits and the effect of additives on surface roughness evolution. One drawback of such Monte Carlo simulations is that they are often characterized by a large number of input parameters, many of which are difficult to quantify experimentally and are thus unknown. Linked calculations were performed on an SGI Power Challenge which supports the parallel MPI (object oriented) architecture used in the finite difference code.

In order to estimate the unknown parameters, a second computational tool was developed to investigate parameter sensitivity and to perform subsequent parameter estimation calculations. The second tool, which consists of multiple linked codes, was used to efficiently determine the unknown input parameters for the Monte Carlo-finite difference simulations. The parameter sensitivity code perturbed all of the input parameters to the Monte Carlo code for a particular additive system to discern which input parameters have the strongest effect on the outputs. The parameter estimation code then tuned these sensitive parameters, compared the simulation outputs with experimental results (scaling parameters obtained from AFM data), then re-tuned the sensitive parameters until the simulation outputs matched the experimental results within a set tolerance. In order to perform the large number of concurrent simulations required to scan large regions of parameter space, simulations were run on a high throughput computing system (linux Condor flock[2]).

A model additive system of chloride (Cl), polyethylene glycol (PEG), and 3-mercapto-1-propane sulfonic acid (MPSA) in acid copper sulfate solution was investigated[3]. The following cases were considered: Cl, MPSA, PEG-Cl, MPSA-Cl, and PEG-Cl-MPSA. Simulations were first performed with the linked Monte Carlo-finite difference code on a flat surface for which experimental (AFM) roughness evolution data are available[4]. The parameter sensitivity code was then used to locate the most sensitive parameters in each case. Next, parameter estimation simulations were run to establish a set of reasonable parameters that describe each case of additive combination that was considered. Finally, the set of parameters obtained from the estimation calculations were used to simulate trench in-fill with the linked Monte Carlo-finite difference codes.

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[1] J. M. E. Harper, C. Cabral Jr., P. C. Andricacos, L. Gignac, I. C. Noyan, K. P. Rodbell, and C. K. Hu, Journal of Applied Physics, 86, 2516 (1999)

[2] For more information see http://www.cs.wisc.edu/condor

[3] T. P. Moffat, J. E. Bonevich, W. H. Huber, A. Stanishevsky, D. R. Kelly, G. R. Stafford, and D. Josell, Journal of the Electrochemical Society, 147(12), 4524-4535, (2000)

[4] J. C. Ganley, Masters Thesis, University of Illinois at Urbana-Champaign (2001)